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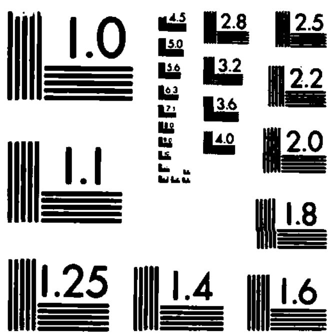

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OPTIMAL CONTROL TECHNIQUES FOR COMPUTING STATIONARY FLOWS OF VISCOELASTIC FLUIDS

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ABSTRACT

~~We~~ document considers the problem of computing the stationary flows of a viscoelastic fluid flowing through a given domain. The proposed numerical method is based on optimal control techniques, which replace the original equations of the problem by a minimization problem to be solved by a descent method. Such techniques are very powerful and can handle equations which change type, provided that, as done here, one uses an adequate preconditioning strategy and that one computes efficiently the gradient of the function to be minimized.

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SIGNIFICANCE AND EXPLANATION

We consider the problem of computing the stationary flows of a viscoelastic fluid flowing through a given domain. The proposed numerical method is based on optimal control techniques, which replace the original equations of the problem by a minimization problem to be solved by a descent method. Such techniques are very powerful and can handle equations which change type, provided that, as done here, one uses an adequate preconditioning strategy and that one computes efficiently the gradient of the function to be minimized.

The responsibility for the wording and views expressed in this descriptive summary lies with MRC, and not with the author of this report.

OPTIMAL CONTROL TECHNIQUES FOR COMPUTING STATIONARY FLOWS OF VISCOELASTIC FLUIDS

Patrick Le Tallec*

1. INTRODUCTION

The objective of this paper is to present from a basic numerical point of view a new class of methods for the numerical calculation of viscoelastic flows. These methods consist in :

(i) rewriting the governing equations as a least-squares problem. Here, it is critical to use the right norms and to introduce a preconditioning operator. For example, working with the quantities $\int_\Omega |\mathrm{div}\, \underset{\sim}{\sigma} - \underset{\sim}{f}\,|^2\, d\underset{\sim}{x}$ is completely inadequate and is wrong from a functional analysis point of view. In this paper, the preconditioning strategy will rely on the introduction of a pivot space;

(ii) solving the resulting minimization problem by a Finite Element Method associated to a conjugate gradient or to a Quasi-Newton algorithm.

This paper first introduces the governing equations of the problem (§2) and rewrites them as a least-squares (or optimal control) problem (§3). The practical calculation of the cost function and of its gradient is then discussed (§4) and several descent methods for solving the resulting minimization problem are presented (§5). Some details on the practical implementation of these ideas and numerical results are finally presented (§6 and §7).

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The framework of the paper will be rather general and could be used for the derivation and the study of different classes of numerical methods. Moreover, although introduced on a standard steady state problem, it can be easily adapted to the solution of true evolution problems, of pseudo evolution problems (time marching techniques) or to an arc length continuation approach (GLOWINSKI [1984, p.206]). In any case, in the proposed methods, approximation errors can be made very small and change of type in the governing equations should not be damaging as seen from the analogy with transonic flow computations.

2. EQUATIONS OF THE PROBLEM

Let us consider a viscoelastic fluid (say of upper-convected Maxwell type), flowing viscously through a given domain Ω (Fig.1). We suppose that no slip occurs along the solid walls and that the fluid velocity at the entrance and at the exit of the domain is given.

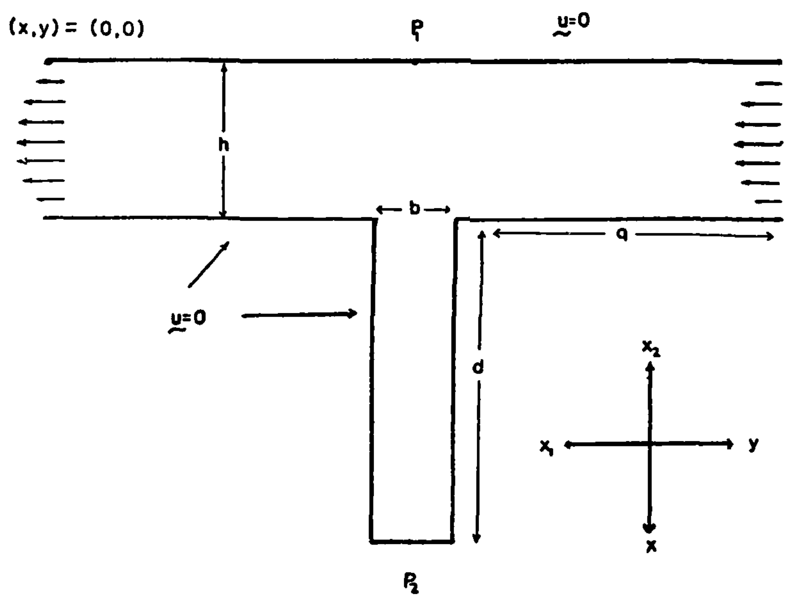


Figure 1 - The physical problem
(out of Malkus [1984])

For example, such situations arise while studying plane flows over slots, such as those studied experimentally by Bird and al. [1982]. The equations governing such situations are simply :

(1) EQUILIBRIUM

$$-\operatorname{div}(\underset{\sim}{\sigma}) + \rho(\underset{\sim}{u}\cdot\underset{\sim}{\nabla})\underset{\sim}{u} = \underset{\sim}{f} \quad \text{in } \Omega ,$$

(2) CONSTITUTIVE LAW (upper-convected Maxwell)

$$\begin{cases} \underset{\sim}{\sigma} = \underset{\sim}{\sigma}_D - p\underset{\sim}{1} , \\ \underset{\sim}{\sigma}_D(\underset{\sim}{x},t) = \int_{-\infty}^{t} \frac{\mu}{\lambda^2} \exp\left(\frac{\tau - t}{\lambda}\right)\left[(\underset{\sim}{F}_t^T\underset{\sim}{F}_t)^{-1} - \underset{\sim}{1}\right] d\tau , \\ \underset{\sim}{F}_t(\underset{\sim}{x},\tau) = \dfrac{\partial X_t(\underset{\sim}{x},\tau)}{\partial \underset{\sim}{x}} , \\ X_t(\underset{\sim}{x},\tau) = \text{position at } \tau \text{ of the particle which is in } \underset{\sim}{x} \text{ at time} \\ \qquad\qquad t \text{ and which is subjected to the velocity field } \underset{\sim}{u}. \end{cases}$$

(3) KINEMATIC RESTRICTIONS

$$\operatorname{div} \underset{\sim}{u} = 0, \quad \underset{\sim}{u} = \underset{\sim}{u}_1 \quad \text{on } \Gamma .$$

Above, $\underset{\sim}{u}$ represents the fluid velocity, $\underset{\sim}{\sigma}$ the Cauchy stress tensor, p a hydrostatic pressure, ρ the fluid density, μ the fluid viscosity and λ the relaxation time. Observe that, as an extra boundary condition, the constitutive law (2) requires the knowledge of what happened to the fluid before it enters the domain.

It has been observed in Joseph, Renardy, Saut [1984], that <u>these equations change type</u> when the viscoelastic Mach number $U/\sqrt{\mu/\lambda\rho}$ reaches 1 (U is a characteristic velocity of the considered flow). Real characteristics then appear along which the vorticity can be discontinuous. However, <u>most numerical methods</u> employed for solving (1)-(3) (such as the classical fixed point method solving iteratively for the velocities and then for the stresses) <u>cannot handle this change of type</u>.

The idea of this paper is to employ for the numerical solution of (1)-(3) optimal control techniques in a dual space, which were used with success in transonic flow computations (GLOWINSKI [1984]), where a similar change of type occurs.

3. LEAST-SQUARES FORMULATIONS OF THE PROBLEM.

3.1. A one-dimensional model problem. Let $f : \mathbb{R} \to \mathbb{R}$ be differentiable and consider the problem of solving numerically the nonlinear equation

$$f(x) = 0 .$$

If it has a solution in $\mathbb{R}$, then this equation is equivalent to

$$\underline{\text{Minimize}}\ \frac{1}{a}|f(x)|^2\ \underline{\text{over}}\ \mathbb{R}, \quad (a > 0) ,$$

problem which can be numerically solved by the gradient algorithm

$$+\ x_0 = \text{given} ,$$

$$+\ \text{for} \quad n = 0 \quad \text{until satisfied set}$$

$$x_{n+1} = x_n - \frac{2}{a} f(x_n)f'(x_n) .$$

This algorithm can be a very efficient method for solving $f(x) = 0$, provided that a is properly chosen and that $f(x)f'(x)$ is easy to compute. It will be the basis of the numerical technique that we will use to solve (1)-(3).

3.2. Maxwell viscoelasticity in primal variables. Let V be the space for the unknown velocity. Here, we take

$$V = \{\underset{\sim}{w} \in \underset{\sim o}{H}^1(\Omega) , \quad \text{div}\ \underset{\sim}{w} = 0\} ,$$

whose topological dual we denote by V^*. Let us also introduce the auxiliary unknown $\underset{\sim}{z} = P\underset{\sim}{u}$, P being a given isomorphism from V onto a Hilbert space H, H with scalar product (.,.) and H identified to its dual. The interest of the auxiliary unknown is that, for P properly chosen, the viscoelastic problem may be better conditioned with respect to this new unknown, and therefore easier to solve numerically. In other words, P is a preconditioning operator. For example, one can think of defining $P\,\mathbf{u}$ as curl $\mathbf{u}$, H as the image of V by P and $(.,.)$ as the L^2 scalar product. The vorticity curl $\mathbf{u}$ will then be the primary variable, which might be a very good choice because vorticity is the canonical variable appearing in the analysis of change of type. Another choice of P, for which again $P^T P$ is equal to the Stokes operator, will be proposed at the finite element level in §5.

Finally, once V and P defined, let us introduce

$$L : V \to \mathbb{R}, \quad L(\mathbf{w}) = \int_\Omega \mathbf{f}.\mathbf{w}d\mathbf{x} ,$$

$$\begin{cases} T : V \to V^*, \\ < T(\mathbf{u}_o), \mathbf{w} > = \int_\Omega \{\rho(\mathbf{u}.\nabla)\mathbf{u}.\mathbf{w} + \frac{1}{2}\,\boldsymbol{\sigma}_D(\mathbf{u}).(\nabla\mathbf{w} + \nabla\mathbf{w}^T)\}\ d\mathbf{x} , \\ \qquad \forall\mathbf{w} \in V,\ \mathbf{u} = \mathbf{u}_1 + \mathbf{u}_o,\ \boldsymbol{\sigma}_D(\mathbf{u}) \text{ being given} \\ \qquad \text{through the constitutive relation (2).} \end{cases}$$

With these notations, summarized in the following diagram

$$\begin{tikzcd} V \arrow[rr, "T"] \arrow[dr, "P"'] & & V^* \ni L \\ & H \arrow[ur, "P^T"'] & \end{tikzcd}$$

equations (1) to (3) take the form

(4) $$T(\mathbf{u} - \mathbf{u}_1) - L = 0 \text{ in } V^* , \quad \mathbf{u} - \mathbf{u}_1 \in V .$$

If (4) has a solution, then it is obviously equivalent to the H <u>least-squares formulation</u> :

$$\boxed{\begin{array}{l} \underline{\text{MINIMIZE}} \quad J(\underset{\sim}{v}) = \frac{1}{2}\,(P\underset{\sim}{y}(\underset{\sim}{v}),\ P\underset{\sim}{y}(\underset{\sim}{v}))\ \underline{\text{OVER}} \quad H \\ \underline{\text{WHERE}} \quad \underset{\sim}{y}(\underset{\sim}{v}) \in V \ \ \underline{\text{IS THE SOLUTION OF THE LINEAR PROBLEM}} \\ \qquad (P\underset{\sim}{y}(\underset{\sim}{v}),\ P(\underset{\sim}{w})) = \langle T(P^{-1}\underset{\sim}{v}), \underset{\sim}{w}\rangle - L(\underset{\sim}{w}),\ \forall \underset{\sim}{w} \in V. \end{array}} \tag{5}$$

Indeed, if (4) has a solution $\underset{\sim}{u}_o = \underset{\sim}{u} - \underset{\sim}{u}_1$, and if we set $\underset{\sim}{v} = \underset{\sim}{z}_o = P(\underset{\sim}{u}_o)$ in (5), then the right-hand side of (5) is equal to zero, thus the associated state vector $\underset{\sim}{y}(\underset{\sim}{z}_o)$ is also equal to zero and therefore $J(\underset{\sim}{z}_o)$ is equal to zero. Since, by definition, J(.) is always positive on H, this implies that $\underset{\sim}{z}_o$ is a minimizer of J over H.

Conversely, let $\underset{\sim}{z}_o$ be a minimizer of J over H. As seen above, since (4) has a solution, J attains the value 0 on H and therefore $J(\underset{\sim}{z}_o)$ must be equal to 0. By definition of J, this can only happen if $\underset{\sim}{y}(\underset{\sim}{z}_o)$ is equal to 0, that is if $T(P^{-1}\underset{\sim}{z}_o) - L = 0$ in V*, which means that $P^{-1}(\underset{\sim}{z}_o)$ is then a solution of (4).

In summary, if we assume the existence of a solution to our original problem (1)-(3), we can replace these equations by the equivalent minimization problem just written above. This minimization formulation is the one which will be used in our numerical techniques. It reduces our initial problem to an optimal control problem, if we identify $\underset{\sim}{v}$ to a control variable, $\underset{\sim}{y}$ to a state vector, (5) to a state equation and J(•) to a cost function.

Here, the state vector belongs to the velocity space, which relates to some extend this formulation to the one used by TANNER [1985], or by the other authors for which the velocity is the working variable.

3.3. Arclength continuation in mixed variables. To illustrate the many directions in which the above optimal control framework can be applied, we will briefly and formally discuss another least squares formulation of problem (1)-(3). It is based on the approach of CROCHET and al [1985] or of BERIS, AMSTRONG and BROWN [1985], among others, in which the original problem is written in mixed variables (velocity + added stress) and is put inside an arclength continuation framework.

With the notations of §3.2, let us first introduce the space Σ of added-stress fields, the space X of trial functions and the operator T_m from $\mathbb{R} \times V \times \Sigma$ into $V^* \times X^*$, respectively defined by

$$\Sigma = \{\tau \in H^1(\Omega),\ \tau = 0 \text{ on } \Gamma^-\},$$

$$X = \{\tau \in H^1(\Omega),\ \tau = 0 \text{ on } \Gamma^+\},$$

$$\Gamma^-(\text{resp. } \Gamma^+) = \{x \in \Gamma, u_1(x) \cdot n(x) < 0 \ (\text{resp.} > 0)\},$$

$$< T_m(\lambda, u_o, \sigma_o), (v, \tau) > = \int_\Omega \{ (\rho(u.\nabla)u - f) \cdot w + \frac{1}{2}\, \sigma_D \cdot (\nabla w + \nabla w^T)$$

$$+ \sigma_D \cdot (-\lambda(u.\nabla)\tau - \lambda(\nabla u)^T \tau - \lambda \tau(\nabla u)) + (\sigma_D - \mu(\nabla u + \nabla u^T)) \cdot \tau \} dx$$

$$+ \int_{\Gamma^-} \lambda \tau \cdot \sigma_D \ u.n \ da, \quad \forall \{w, \tau\} \in V \times X,$$

with $u = u_o + u_1$, $\sigma_D = \sigma_o + \sigma_1 + \mu(\nabla u + \nabla u^T)$, u_1 and σ_1 corresponding to the given boundary velocities and input added stresses.

Now, following the strategy of CROCHET [1985], writing the constitutive law under a differential form and integrating by parts, the arclength continuation problem associated to (1)-(3) can be written :

$$(6) \begin{cases} \underline{\text{Find}} \ \{u_o, \sigma_o, \lambda\} : [0,S] \to V \times \Sigma \times \mathbb{R} \ \ \underline{\text{such that}} : \\ \lambda(0) = 0, \ \sigma_o(0) = 0, \ u_o(0) + u_1 = \text{Stokes solution;} \\ < T_m(\lambda(s), u_o(s), \sigma_o(s)), (w, \tau) > = 0, \forall \{w, \tau\} \in V \times X, \ \forall s \in [0,S] ; \\ \left|\frac{d}{ds}(P\, u_o)\right|_H^2 + \left|\frac{d}{ds}(\sigma_o)\right|_{H^1(\Omega)}^2 + \left(\frac{d}{ds}\lambda\right)^2 = 1. \end{cases}$$

After discretization in s, we obtain

$$\begin{cases} \forall n>0, \ \underline{\text{find}} \ \{\underset{\sim}{u}_o^n, \underset{\sim}{\sigma}_o^n, \lambda^n\} \in V \times \Sigma \times \mathbb{R} \ \underline{\text{such that}} \\ < T_m(\lambda^n, \underset{\sim}{u}_o^n, \underset{\sim}{\sigma}_o^n), (\underset{\sim}{w}, \underset{\sim}{\tau}) > = 0, \quad \forall \{\underset{\sim}{w}, \underset{\sim}{\tau}\} \in V \times X, \\ (P \underset{\sim}{u}_o^n - P \underset{\sim}{u}_o^{n-1}, P \underset{\sim}{u}_o^{n-1} - P \underset{\sim}{u}_o^{n-2}) + (\underset{\sim}{\sigma}_o^n - \underset{\sim}{\sigma}_o^{n-1}, \underset{\sim}{\sigma}_o^{n-1} - \underset{\sim}{\sigma}_o^{n-2}) \\ + (\lambda^n - \lambda^{n-1})^2 = \Delta s^2, \end{cases}$$

from which we derive our final least-squares formulation of the arclength continuation problem

$$(7) \begin{cases} \forall \ n>0, \ \underline{\text{Minimize the cost function}} \ \text{(residual dual norm)} \\ J(\lambda, \underset{\sim}{z}_o, \underset{\sim}{\sigma}_o) = \frac{1}{2} |P\underset{\sim}{y}|_H^2 + \frac{1}{2} |\underset{\sim}{\sigma}^*|_{H^1}^2 + \frac{1}{2} \mu^2 \\ \underline{\text{over the control space}} \ \mathbb{R} \times H \times \Sigma, \ \underline{\text{the state vector}} \ \text{(residual)} \ \{\underset{\sim}{y}, \underset{\sim}{\sigma}^*, \mu\} \\ \underline{\text{in}} \ V \times X \times \mathbb{R} \ \underline{\text{being defined through the state equation}} \\ (P\underset{\sim}{y}, P\underset{\sim}{w})_H + (\underset{\sim}{\sigma}^*, \underset{\sim}{\tau})_{H^1} = < T_m(\lambda, P^{-1}\underset{\sim}{z}_o, \underset{\sim}{\sigma}_o), (\underset{\sim}{w}, \underset{\sim}{\tau})>, \ \forall \{\underset{\sim}{w}, \underset{\sim}{\tau}\} \in V \times X, \\ \mu = \Delta s^2 - (\lambda - \lambda^{n-1})^2 - (\underset{\sim}{z}_o - \underset{\sim}{z}_o^{n-1}, \underset{\sim}{z}_o^{n-1}, \underset{\sim}{z}_o^{n-2}) - (\underset{\sim}{\sigma}_o - \underset{\sim}{\sigma}_o^{n-1}, \underset{\sim}{\sigma}_o^{n-1} - \underset{\sim}{\sigma}_o^{n-2}) . \end{cases}$$

Observe that (7), as it must do, deals with the right dual norms of the residuals, and that it is in fact equivalent to the standard discretizations of (6) used in the litterature.

4. CALCULATION OF THE COST FUNCTION AND OF ITS GRADIENT

The minimization formulations of §3, although equivalent to classical ones, are very interesting because they can be solved by a different class of stable numerical algorithms. Indeed, any available descent method (conjugate gradient, Buckley-Lenir, Quasi-Newton...) can be successfully used for their numerical solution. The practical implementation of such methods only requires the knowledge, at given controls $\underset{\sim}{v}$, of the cost function $J(\underset{\sim}{v})$ and of its gradient $J'(\underset{\sim}{v})$.

Now, the cost function being a quadratic function of the state vector, the latter being the image of a nonlinear complicate operator acting on the control vector, the computation of J or of J' is not an easy matter. Nevertheless, even in the more complex situation of §3.2, and unlike a classical Newton method which would require $O(N^3)$ operations (N=dim V) to compute this gradient, the computation of J' can be done in $O(N^2)$ operations by introducing an adjoint state vector which reduces this computation to the explicit integration of functions locally defined on the support of each trial function.

To see that, in the framework of §3.2, let us introduce the adjoint state $\underset{\sim}{G}(\underset{\sim}{v})$ defined as

$$(8)\qquad \underset{\sim}{G}(\underset{\sim}{v})(\underset{\sim}{x},t) = \frac{1}{\lambda}\int_{-\infty}^{t} \exp\left(\frac{\tau - t}{\lambda}\right)(\underset{\sim}{F}_t^-(\underset{\sim}{x},\tau))^T \underset{\sim}{D}(X_t^-(\underset{\sim}{x},\tau))\underset{\sim}{F}_t^-(\underset{\sim}{x},\tau)d\tau ,$$

with

$$(9)\qquad \begin{cases} \underset{\sim}{D} = \frac{1}{2}\,(\nabla\underset{\sim}{\chi}(\underset{\sim}{v}) + (\nabla\underset{\sim}{\chi}(\underset{\sim}{v}))^T) \quad \text{if} \quad \underset{\sim}{x} \in \Omega , \\ \underset{\sim}{D} = 0 \quad \text{if} \quad \underset{\sim}{x} \notin \Omega , \\ \underset{\sim}{F}_t^-(\underset{\sim}{x},\tau) = \dfrac{\partial X_t^-}{\partial \underset{\sim}{x}}(\underset{\sim}{x},\tau) , \\ X_t^-(\underset{\sim}{x},\tau) = \text{position at time } \tau \text{ of the particle which} \\ \qquad\qquad \text{is in } \underset{\sim}{x} \text{ at time } t \text{ and which is subjected} \\ \qquad\qquad \text{to the velocity field } \underset{\sim}{u}^-(\underset{\sim}{x}) = -\underset{\sim}{u}(\underset{\sim}{x}). \end{cases}$$

This adjoint state can be computed by an explicit integration along the trajectories of $\underset{\sim}{u}=P^{-1}(\underset{\sim}{v})+\underset{\sim}{u}_1$. Then, we can prove

<u>THEOREM</u> : <u>The gradient</u> $J'(\underset{\sim}{v})$ <u>is the solution of the linear problem</u>

$$(10)\qquad (J'(\underset{\sim}{v}),\ P\underset{\sim}{w}) = \int_\Omega \rho\{(\underset{\sim}{w}.\underset{\sim}{\nabla})\underset{\sim}{u} + (\underset{\sim}{u}.\underset{\sim}{\nabla})\underset{\sim}{w}\}.\underset{\sim}{\chi}(\underset{\sim}{v})d\underset{\sim}{x}$$

$$+\int_\Omega \{\mu(\nabla\underset{\sim}{w} + \nabla\underset{\sim}{w}^T) + \lambda(\nabla\underset{\sim}{w})\underset{\sim}{\sigma}_D + \lambda\underset{\sim}{\sigma}_D(\nabla\underset{\sim}{w})^T - \lambda(\underset{\sim}{w}.\underset{\sim}{\nabla})\underset{\sim}{\sigma}_D\}.\underset{\sim}{G}(\underset{\sim}{v})d\underset{\sim}{x},\forall\underset{\sim}{w}\in V.$$

<u>Proof</u> : By definition of the gradient, we have

$$(J'(\underset{\sim}{v}),\underset{\sim}{z}\ ) = \lim_{t\to 0}\frac{1}{t}\,[J(\underset{\sim}{v} + t\underset{\sim}{z}) - J(\underset{\sim}{v})] = (P\underset{\sim}{\chi},\ P\delta\underset{\sim}{\chi})$$

where $\chi = \chi(v)$ is the solution of the state equation (5) and where $\delta\chi$ is obtained from z by differentiation of (5), that is by solving

$$(P\delta\chi,\ Pw) = \langle T'(P^{-1}v).P^{-1}z,\ w\rangle,\ \forall w \in V .$$

Substituting this definition of $\delta\chi$ in the expression of the gradient, we get

$$(J'(v),z) = \langle T'(P^{-1}v).P^{-1}z,\ \chi\rangle.$$

Denoting $P^{-1}z$ by w, and from the definition of $T(.)$, this gives

$$(11)\quad (J'(v),\ Pw) = \int_\Omega \{\rho(w.\nabla)u + \rho(u.\nabla)w\}.\chi dx + \int_\Omega [\sigma_D'(u).w].D(\chi)dx ,$$

with $D(\chi) = \frac{1}{2}(\nabla\chi + \nabla\chi^T)$. In (11), to compute the action of the derivative of $\sigma_D(u)$ on w, we differentiate the constitutive law (2), first with respect to time, then with respect to the velocity u. We obtain

$$(12)\begin{cases} \tau = \sigma_D'(u).w \ \ \underline{\text{satisfies the differential equation}} \\ \lambda\ (u.\nabla)\tau - \lambda(\nabla u)\tau - \lambda\tau(\nabla u)^T + \tau \\ = 2\mu D(w) - \lambda(w.\nabla)\sigma_D(u) + \lambda(\nabla w)\sigma_D(u) + \lambda\sigma_D(u)(\nabla w)^T , \\ \tau = 0 \quad \text{on } \Gamma^- \ (= \text{part of } \Gamma \text{ with } u_1 \ .\ n < 0). \end{cases}$$

On the other hand, by differentiating the adjoint state equation (8) with respect to time, we have

$$(13)\quad \int_\Omega \tau.D(\chi)dx = \int_\Omega \tau.[-\lambda(u.\nabla)G - \lambda(\nabla u)^T G - \lambda G(\nabla u) + G]dx \quad .$$

Integrating (13) by parts, and taking the incompressibility constraint div $u = 0$ into account, (13) yields

$$\int_\Omega \tau.D(\chi)dx = \int_\Omega G.[\lambda(u.\nabla)\tau - \lambda\tau(\nabla u)^T - \lambda(\nabla u)\tau + \tau]dx$$

which from (12) is equivalent to

$$(14)\quad \int_\Omega \tau.D(\chi)dx = \int_\Omega G.\{2\mu D(w) - \lambda(w.\nabla)\sigma_D + \lambda(\nabla w)\sigma_D + \lambda\sigma_D(\nabla w)^T\}dx .$$

Plugging (14) back in (11) finally gives (10) and our proof is complete. □

With this theorem, the computation of $J(\underset{\sim}{v})$ and $J'(\underset{\sim}{v})$ reduces to the following sequence of operations.

$$\left\{\begin{array}{ll}
\text{(i)} & \text{Solve } \; P\underset{\sim}{w} = \underset{\sim}{v} \; \text{ in } H,\ \underset{\sim}{w} \in V\ ; \\
\text{(ii)} & \text{Compute } \underset{\sim}{\sigma}_D(\underset{\sim}{w}+\underset{\sim}{u}_1) \text{ by integration of the constitutive law (2) ;} \\
\text{(iii)} & \text{Compute the right-hand side } \underset{\sim}{r} \text{ of the state equation (5);} \\
\text{(iv)} & \text{Compute the state vector } \underset{\sim}{y} \text{ by solving the linear problem (5) ;} \\
\text{(v)} & J(\underset{\sim}{v}) = \frac{1}{2}\,(P\underset{\sim}{y},\ P\underset{\sim}{y}) = \frac{1}{2} < \underset{\sim}{r},\ \underset{\sim}{y} > \ ; \\
\text{(vi)} & \text{Compute the adjoint state } \underset{\sim}{G} \text{ by integration of (8);} \\
\text{(vii)} & \text{Compute the right-hand side } \underset{\sim}{j} \text{ of the gradient equation (10) ;} \\
\text{(ix)} & \text{Compute } J'(\underset{\sim}{v}) \text{ by solving the linear problem (10).}
\end{array}\right.$$

In summary, for the least squares formulation (5), the computation of J and of J' requires two integrations in time and the solution of four linear problems associated to the fixed operators P or P^T.

5. A TYPICAL CHOICE FOR THE DESCENT METHOD AND FOR THE PRECONDITIONING OPERATOR

We still consider the framework of §3.2 and we now suppose that V is approximated by a finite dimensional space V_h with basis $(\underset{\sim}{\varphi}_i)i=1,N$, to which we associate the matrix.

$$A=(A_{ij})_{i=1,N,j=1,N}\ ,\ A_{ij}=\int_\Omega 2\,\mu\ \underset{\sim}{D}(\underset{\sim}{\varphi}_i)\cdot\underset{\sim}{D}(\underset{\sim}{\varphi}_j)d\underset{\sim}{x}\ .$$

We then define P as the Choleski factorization of A ($P^TP=A$, P lower triangular), H as $\mathbb{R}^N$ and (.,.) as the canonical scalar product on $\mathbb{R}^N$.

With this choice of P and H, the minimization problem (5) can be solved by the standard Polak Ribière conjugate gradient method given below :

x $\underset{\sim}{v}^o$ given ;

x $\underset{\sim}{g}^o = J'(\underset{\sim}{v}^o)$ as computed in §4 ;

x $\underset{\sim}{w}^o = \underset{\sim}{g}^o$;

for $n \geq 0$, with $\underset{\sim}{v}^n$ and $\underset{\sim}{w}^n$ known, and until satisfied, do :

x solve $J(\underset{\sim}{v}^n - \rho_n \underset{\sim}{w}^n) \leq J(\underset{\sim}{v}^n - \rho \underset{\sim}{w}^n)$, $\forall \rho \in \mathbb{R}$, $\rho_n \in \mathbb{R}$,

(use quadratic interpolation, for example)

x $\underset{\sim}{v}^{n+1} = \underset{\sim}{v}^n - \rho_n \underset{\sim}{w}^n$,

x $\underset{\sim}{g}^{n+1} = J'(\underset{\sim}{v}^{n+1})$ as computed in §4 ,

x $\underset{\sim}{w}^{n+1} = \underset{\sim}{g}^{n+1} + \underset{\sim}{w}^n (\underset{\sim}{g}^{n+1}, \underset{\sim}{g}^{n+1} - \underset{\sim}{g}^n)/(\underset{\sim}{g}^n, \underset{\sim}{g}^n)$.

The numerical results given below were obtained by solving (5) with this Polak-Ribière algorithm. To accelerate convergence, we have recently replaced this algorithm by the one described in BUCKLEY and LENIR [1983], which begins by a few steps of a BFGS method and which then switches to a conjugate gradient method using the last BFGS update of the Hessian as an additional preconditioning matrix. Again, the practical implementation of this last method only requires the knowledge of J and J', as obtained from §4, and only involves the solution of linear systems which are associated to fixed positive definite symmetric sparse matrices and which are thus cheap to solve even for N large. On (5), this last algorithm gives comparable results but appears more robust than the original Polak-Ribière method.

6. NUMERICAL IMPLEMENTATION

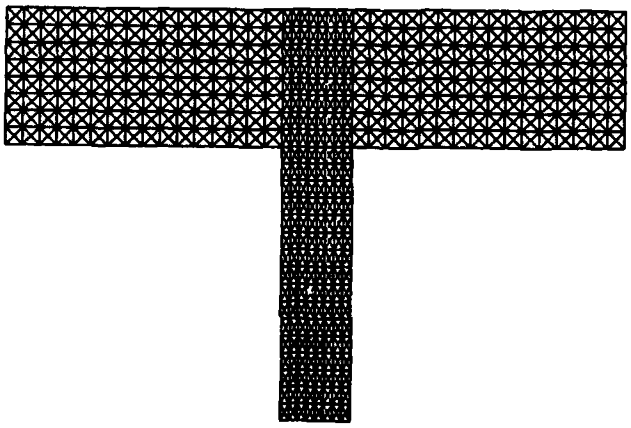
In the framework of §3.2, the implementation on a computer of the techniques of §4 and §5 requires the solution of two numerical problems :

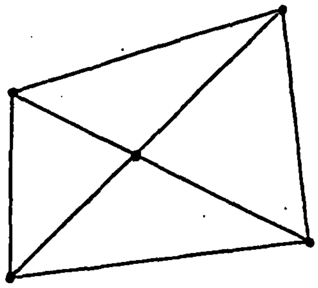
(i) what type of approximation can be used for the space V of velocity fields ?

(ii) for a given velocity field, what numerical technique can be used for the integration in time of the constitutive law and of the adjoint state equation?

Those problems are strongly interconnected since, for example, the finite element which is used determines the aspect of the computed trajectories. D. Malkus [1984] proposes answers which are very attractive because they respect the physical structure of the problem. His technique decomposes as follows :

(i) choice of an exactly incompressible piecewise linear finite element (such as the linear crossed triangle) for approximating the velocity field;





The original piecewise linear Finite Element made of four linear crossed triangles.

Mesh of the domain.

Figure 2 - Linear Crossed Triangles

(ii) exact computation of the trajectories incoming at the center of each finite element through a piecewise analytical solution of the ordinary differential equation

$$\dot{X}_t(\underset{\sim}{x},\tau) = \underset{\sim}{u}[X_t(\underset{\sim}{x},\tau)] , \quad X_t(\underset{\sim}{x},t) = \underset{\sim}{x} ;$$

(iii) computation of the deformation gradient history by solving analytically the equation

$$\dot{\underset{\sim}{F}}_t(X_t(\underset{\sim}{x},\tau)) = \underset{\sim}{\nabla u}[X_t(\underset{\sim}{x},\tau)]\underset{\sim}{F}_t(X_t(\underset{\sim}{x},\tau)), \quad \underset{\sim}{F}_t(\underset{\sim}{x},t) = \underset{\sim}{1} ;$$

(iv) computation of the added stresses $\underset{\sim}{\sigma}_D$ by a Laguerre type numerical quadrature

$$\underset{\sim}{\sigma}_D(\underset{\sim}{x},t)=\int_{-\infty}^{t} m_1(\tau)\ [\underset{\sim}{F}_t(\underset{\sim}{x},\tau)]\ d\tau \approx \sum_{i=1}^{NT} W(\tau_i)m_1(\tau_i)\ (F_t(\underset{\sim}{x},\tau_i))\ .$$

The numerical quadrature of (iv) slightly changes the constitutive law but respects its objectivity since the trajectories and deformation gradients are exactly computed.

For a viscoelastic fluid with a more complicated differential constitutive law, the Laguerre quadrature is replaced by a forward numerical integration of the constitutive law on the computed trajectories, using an automatic time stepping strategy. In the case of an evolution problem, the integration in (iv) is only performed between times t_n and t_{n+1}, which is then much cheaper.

In summary, if we use D. Malkus ideas, our numerical technique for the solution of (1)-(3) finally reduces to

1) the transformation of the original equations (1)-(3) into an equivalent *minimization formulation* (§3).

2) the solution of this minimization problem by a standard descent technique (§5),

3) the approximation of the velocity fields by linear crossed - triangular finite elements (§6),

4) the construction of a preconditioning operator by a Choleski factorization of the Stokes operator,

5) the numerical integration of the constitutive laws by a numerical quadrature on the analytically computed trajectories (§6).

As described the method is expected to be stable, even if there is change of type (this is typical of a dual least-squares approach), and accurate (very little approximation appears in the integration of the constitutive laws).

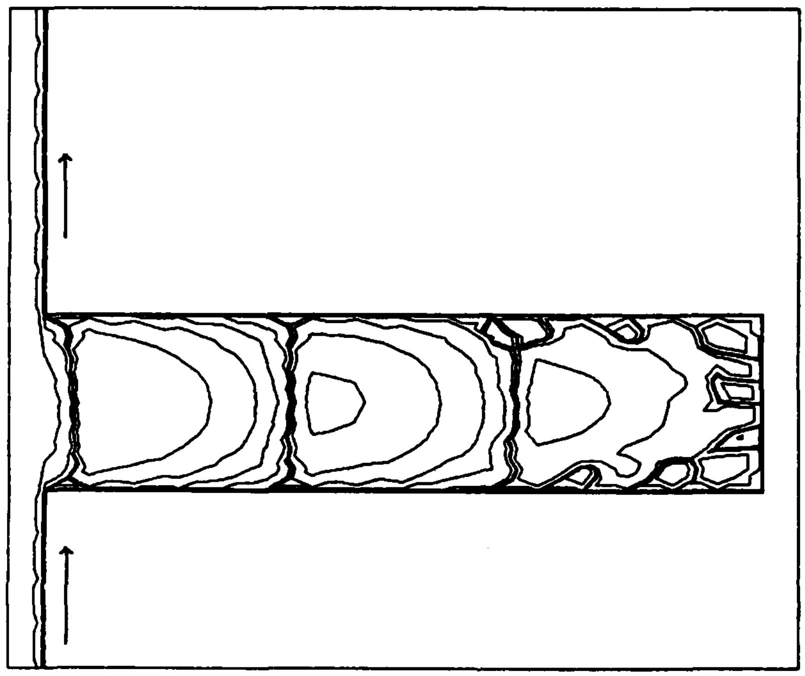
Moreover, although mainly illustrated in the upper-convected Maxwell-case, the method can be applied to any constitutive model which reduces to a differential equation. In particular, for such models, the gradient $J'(.)$ can still be computed as in §4, simply by replacing (13) by the transpose of the differential equation defining $\underset{\sim}{\sigma}'_D(\underset{\sim}{u}).\underset{\sim}{w}$.

Nevertheless, the method appears to be very expensive, especially in the steady case where almost all the computation time is used for the exact calculation of the trajectories at a given velocity field. In that respect, the mixed formulation of §3.3 appears more attractive because there no such calculation is needed.

7. NUMERICAL RESULTS

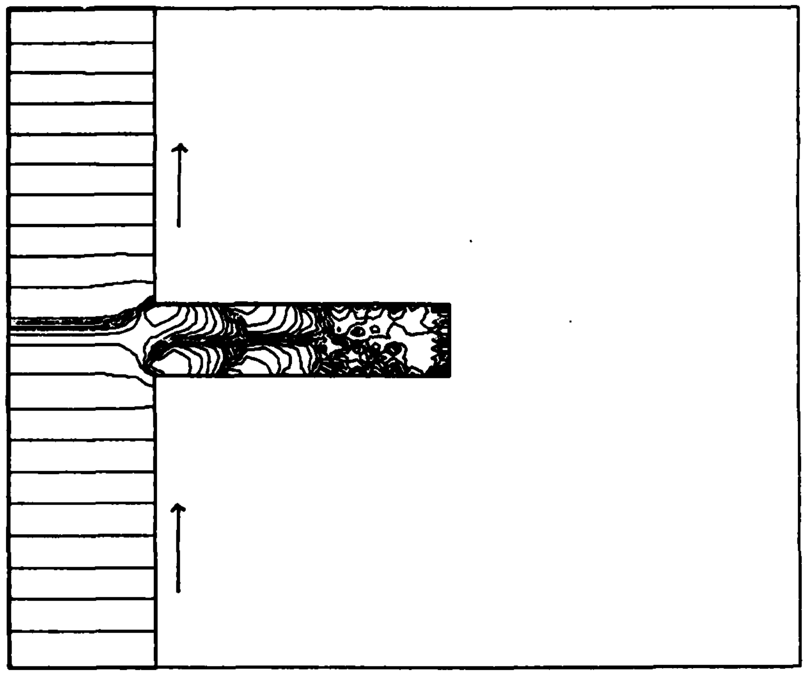
We consider below the numerical study of the plane stationary flow over a slot of an upper-convected Maxwell fluid. The domain and the boundary conditions of the flow are those of Fig.1, and its associated Deborah and Reynolds number are respectively De=.75 and Re=.86 10^{-4} (Deborah number = product of the fluid relaxation time by the shear rate of the incoming fluid at the solid wall). The aspect of the streamlines inside the slot and of the hydrostatic pressure profiles are represented on Fig.3 and 4.

The computation was done on a Cray 1, with the finite element mesh represented on Fig.2 (961 nodes), and using the Polak-Ribière algorithm of §5. Fifteen iterations were required for an execution time of 12 mn. More than 95% of this time was devoted to the analytical computation of the trajectories, to be done twice per iteration. This indicates that our strategy for the computation of the trajectories should be revisited in the stationary case, and that it may be better there to use the mixed formulations of §3.3.



SLOT
DE = .75 , RO = .332338e-3
Iteration 15

Figure 3 - Streamlines inside the slot (rising flow)



SLOT pression
DE = .75 , R_e = .000332338
iteration 15

Figure 4 - Hydrostatic pressure profiles
(rising flow)

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We consider the problem of computing the stationary flows of a viscoelastic fluid flowing through a given domain. The proposed numerical method is based on optimal control techniques, which replace the original equations of the problem by a minimization problem to be solved by a descent method. Such techniques are very powerful and can handle equations which change type, provided that, as done here, one uses an adequate preconditioning strategy and that one computes efficiently the gradient of the function to be minimized.

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